A COMPUTER PROGRAM FOR FILTER MEDIA DESIGN OPTIMIZATION

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A COMPUTER PROGRAM FOR FILTER MEDIA DESIGN OPTIMIZATION

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Thesis

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ABSTRACT

In depth filtration, mixtures of nanofibers and microfibers provide efficient and effective filters for capture of micron and submicron sized particles. Experimental approaches are time consuming and expensive to design filters. There is a need for reliable computational models to analyze and evaluate the filter performance. The objective of this research is to present a computational approach for designing mixed fiber filter media for depth filtration. The goal is to find an optimum solution, given specified ranges for a set of design parameters: thickness of the media, diameter of microfiber, diameter of nanofiber, surface area ratio of nanofiber to microfiber, and mass of microfiber. The idea is to develop with a software tool that may reduce the number of experiments.

This program applies a Genetic Algorithm to search for an optimum filter media design based on Quality Factor which quantifies the filter performance. A user friendly computer program is developed that provides inputs, outputs and controls to design a filter media. This program provides a starting point for design of filter media for particular applications.

Experiments were performed to validate the modeling and experimental data for comparison. The results show about 25% error in quality factor between computer model and experiments. More experiments are needed in future work for model validation.

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CHAPTER I

INTRODUCTION

1.1 Background information

In many industrial sectors fibrous filters are used to remove undesirable particles from gas streams. These filters are used in nuclear, pharmaceuticals, chemical industry, power generation, food processing and beverage industry, electronics, biotechnology, mining and the pulp and paper industries [1].

Micron and submicron sized particles in air are commonly known to be harmful to human health and to the environment. One method to remove these particles from aerosols is by non woven microfiber filters. The performance of a fibrous filter media is dependent upon the size of particles to be filtered, the structure of the filter media, such as fiber diameter, the packing density, filter thickness, filtration velocity, and the viscosity, pressure and temperature of the gas. The addition of nanofibers to the microfiber media improves the filter performance but design correlations for the relative amounts of nanofibers to add to the fiber mixture are not commonly available.

In this thesis a computer program is developed that searches for the best values, within specified ranges, of five design parameters of filter media that optimizes the filter performance. The filter performance is defined by the quality factor which is given by R.C.Brown[2] which accounts for capture efficiency and pressure drop. The higher the quality factor the better the filter performance.

The computer program is named FiL2RO (pronounced "fill too rho") which is an acronym for "<u>Fi</u>lter Media <u>L</u>ocal Mechanism <u>2</u> Fibe<u>r</u> <u>O</u>ptimization." The governing equations solved by the program are based on volume averaged continuum theory species and momentum balances. Local single fiber mechanisms for particle capture and drag force are used to model the interphase terms in the equations. The program assumes the particles to be captured are monodispersed and the filter is clean (*ie.* no particles are loaded into the medium). The program allows the user to select two fiber sizes for which the fibers are mixed together to form the medium. The porosity of the medium is calculated for the optimum design and is large (greater than 0.9) making the local single fiber mechanism assumptions reasonable.

1.2 Research Objectives

- 1. Develop a computational model to predict the filter performance for depth filtration.
- 2. Selection of design parameters of filter media for optimization.
- 3. Develop a software program to find optimum parameter values of mixed fiber filter media design using the Genetic Algorithm search technique.
- 4. Selection of fitness function and convergence criterion.
- 5. Interpret and analyze the results from the software program.

- 6. Construct and test filters to measure quality factor with varying amounts of nanofibers in glass fiber media.
- 7. Compare model calculations with experimental data.
- 8. Compare optimum filter performance with optimization program.

1.3 Technological importance

This work shows that existing correlations can be applied with the volume averaged continuum equations to predict performance trends in filter media. The computer program can reduce the number of laboratory trial runs of making and testing filter media. The program can help in studying the trends or improvements in making filter media that would be costly to find using traditional or experimental methods. We can predict the effects of filtration properties of non-woven filter media on filter performance and its efficiency. This work can be extended to quantify the efficiency of filters for layers of media with different structures.

1.4 Thesis Outline

The thesis is structured into six chapters. The second chapter contains literature review explaining about the aerosol filters, fibrous filters, characteristics of fibrous filter, simulation models, introduction to search technique Genetic Algorithm and importance of nanofiber in filtration. The third chapter explains about the model background, particle capture mechanism, assumptions, and the equations used to develop filter design optimization program and model results. Chapter 4 explains about the software program written in FORTRAN and Visual Basic user interface, inputs and output parameters, features and limitations of the program. Chapter 5 describes the media preparation and characterization of media. Sixth chapter explain about the coalescence experiments and the results. Chapter 7 has conclusion and future work followed by appendices.

CHAPTER II

LITERATURE REVIEW

2.1 Methods of filtration

The filtration of fine particles and contaminants present in gases that originate from process industries, automotive, healthcare, aerospace is paramount to health and environment [3].





The particles can be removed by filter media in two methods namely Surface and Depth filtration, as shown in Figure 2.1. In this review, the focus is on depth filtration. Surface filtration is common in filtration of gases with high particle concentrations. Depth filtration is most commonly applied to low concentrations of particles in gases to reduce particle concentrations to very low levels.

1. Surface Filtration

Surface filtration traps contaminants larger than the pore size on the top surface of the media forming a filter cake [4]. Contaminants smaller than the pore size may pass through the filter. Mechanisms such as bridging may capture some of the particles smaller than the pore size on the filter surface. These filters are generally polymeric films approximately 120 μ m thick with a narrow pore size distribution. Examples are membrane filters and cloths dryer filter.

2. Depth Filtration

The process of depth filtration allows particles to penetrate into the filter media and get captured throughout the depth of the filter media and on the surface of the media. Depth filters are composed of random mats of metallic, polymeric or inorganic materials. These filters have broad pore size distribution. Examples are fibrous filters and furnace filters.

2.2 Fibrous Filters

As evident from Figure 2.2, contaminant particles range from 0.1 nm to 100 μ m and the most penetrating particle range is between 100 and 500 nm. Fibrous filters are commonly used medium for particles in size ranging from about 0.2 to 500 microns. They are composed of randomly oriented fibers, which may or may not be glued together with a binder. They can be characterized as having low resistance to air flow, low pressure drop and exceptional particle capture capabilities [2]. Fibrous media are widely used in disposable filters, due to relatively low cost with acceptable performance.



Particle size (micrometers)

Figure 2.2 Common air contaminants and their relative sizes [5]

- 2.2.1 Factors effecting particle capture
- 1. Physical properties of Filter media

Physical parameters such as fiber sizes, filter thickness, porosity (void volume), and

solid volume fraction have marked effects on the performance of fibrous filters [3].

The effecting parameters are

- d_i Fiber diameter
- L Filter thickness
- α Projected area of fiber per unit filter area and length of filter
- l_f Fiber length per unit filter surface area

- *S* Packing density (solid volume fraction)
- ε Porosity (void volume fraction)

Some relationship among these parameters are

$$\varepsilon = 1 - \alpha$$
 2.1

$$S = \pi d_i^2 l_f / L \tag{2.2}$$

$$\alpha = 4S/(\pi d_i)$$
 2.3

- 2. Particle characteristics
 - a. Size distribution
 - b. Phase solid/ liquid
- 3. Gas conditions
 - a. Flow rate

The flow per unit area depends largely on the particle size and distribution of the particulates, pressure drop, total porosity and filter area. Generally flow can be maximized by adding filter surface area.

- b. Temperature
- c. Pressure
- d. Viscosity

The viscosity of the material passing through the medium can greatly affect the flow rate, differential pressure and energy cost associated with filtration. 2.2.2 Filter efficiency measurement [6]

1. Pressure Drop

Pressure drop is the difference between the upstream pressure and the downstream pressure. The pressure drop is the most important design feature in the filtration industry and a significant contributor to a systems energy cost. Pressure drop is primarily influenced by the properties of filter media, gas velocity and viscosity.

2. Filter Efficiency Rating

Efficiency can be measured in many ways which includes

a. Beta Ratio

Beta ratio is an efficiency measurement of a filter is expressed as ratio of number of particles of a given size in upstream per unit of volume to the number of particles in downstream of that same size per unit volume. It is expressed as percentage

b. Gravimetric rating

Gravimetric rating is the amount of particles measured as weight in a predetermined volume removed by a filter. It is determined by weighing the solution passing from the upstream to the downstream side.

c. Microbial rating: H.I.M.A. test

Microbial rating is the measure of a filter's ability to sterilize liquids, usually through use of 0.2 micron rated microporous membranes. This liquid challenge procedure is defined as the logarithmic of the ratio of microorganisms upstream to those found downstream and expressed as efficiency as a log reduction value (LRV).

3. Dirt Holding Capacity

The amount of dirt a filter can capture and hold with an acceptable pressure drop is defined as the dirt holding capacity. It is determined by the size of the particulate matter retained as influenced by the size of the pores.

4. Filter rating

Filter rating used to refer to the particle size capture capability of a filter.

5. Useful Life

The useful life of a filter is determined at of the point when particles (contaminants) cause an adverse flow rate, low efficiency, and high pressure drop.

Fibrous filter performance depends on many parameters of filter media. Fiber diameter, fiber cross section and media thickness are the big drivers that effect filter performance. The smaller the fiber diameter, the greater the capture efficiency and the smaller the fiber spacing, the greater the filter efficiency. The larger the cross section, the greater the capture capability [3]. Pressure drop across a filter varies with it thickness, air velocity, the fiber radius and coefficient of viscosity of the air [2]. Media thickness and basis weight influence filter porosity. Fiber diameter and fiber size distribution, pore size influence aerosol flow in the media which play an important role in filter efficiency [4].

The traditional way of making and testing of filters is time consuming and expensive. This is due to highly complex relationship between physical, chemical and geometric properties of individual fibers, physical and chemical properties of gas, and size, mass and shape of dirt particles. Some work has been done to mathematically model the behavior of flow through filter media. The following section reviews selected work.

2.3 Computer models

Several theories on air filtration are described by R.C.Brown [2]. He reviews the single fiber efficiency theory wherein several particle capture mechanism are combined in the capture of a particle. Rosner et al [9] describe the theory of particle on cylindrical surfaces. In the late 1950s, Happel [10,11] and Kuwabara [12] formulated the multifiber filter models. It described the influence of neighboring fibers and employed artificial boundary conditions. Brown [2], in the late 1980's solved the Navier Stokes equation and further advanced the multifiber filtration theory. Liu and Wang (1996) have recently improved the multifiber model to greater degree [13].

Fraunhoffer University had developed many simulation software models; one of them is software simulation of flow through oil filters [14]. It provides evaluation of pressure drop, flow rate ratio before manufacturing a prototype, optimal design of the ribs (supporting the filter medium) on the basis of flow computations and evaluation of uniform loading of the filter medium. The mathematic model, used for filtration simulation, showed excellent efficiency with respect to the analysis of the investigated filtration process. It shows detailed information about velocity and pressure distribution in the filter thus assisting engineers in the design of more efficient filters.

A non woven media model together with the simulation of fluid flow and particle tracking and particle deposition provides deep insights into the filtration processes in complex filter media [15]. Non woven geometries, pressure distribution, local flow velocities and media clogging, filter efficiencies and filter lifetime including pressure drop evolution and filter efficiency over time are visualized and evaluated in this model. The Navier Stokes equation is used to describe the motion of fluid and the flow is computed using an Eulerian model (applying equations from continuum mechanics). The motion and deposition of spherical particles of various sizes is computed by a Lagrangian formulation for the particle motion (*i.e.*, force balances are applied to each particle to model particle-particle and particle-fiber interactions).

Srinivasan [16] investigated the effects of incorporating nanofibers in glass microfiber filter media. In her model volume averaged multiphase transport theory [17] was used to aid the set up the governing equations used to solve the species balance to predict the trend in quality factor of filter media upon addition of nanofibers. The model results show the advantages of adding nanofibers to microfiber filter media [18,19].

Numerical models can significantly reduce the experimental effort of producing new material prototypes [15]. These models have potential to provide valuable insights on how to design new filter media for modern filtration applications as needs arise for separating and filtering particles of different sizes at different operating conditions.

2.4 Optimization Techniques [20]

There are different search optimization techniques like calculus of variation, linear programming, non linear programming and dynamic programming. Calculus of variation is meant only for linear equations. Dynamic programming has difficulty in dimensionality. All these techniques are initial point dependent and it cannot analyze the wide spread solutions. It is not always practical to find global optima using these techniques on large scale problems. Enhancement of these techniques to search for global optima greatly increases computational time with no guarantees that the optimal solutions will be found.

As a compromise to make computational efforts more manageable, other search techniques have been developed such as Evolutionary Algorithms. A Genetic Algorithm (GA) is one such evolutionary algorithm and is used in this work.

Evolutionary algorithms are global optimization techniques for solving large scale problems that have many local optima. However they require high CPU times, and they are very poor in terms of convergence performance. Evolutionary algorithms tend to not get trapped on local minima and can often find global optimal solutions. There are other search techniques like simulated annealing which is a probabilistic search algorithm, tabu search which avoid discrete searches getting stuck in local minima and alpha beta pruning which can be used to search good moves in zero sum games. GAs and Neural Networks have been found to offer advantages over conventional methods, for those involving non linear and complex mathematical relations [21].

GAs were invented by John Holland and his student in 1975. The GA introduces the principle of evolution and genetics into search among possible solutions to a given problem. The idea is to simulate the process in natural systems. This is done by an iterative procedure that consists of fixed population of possible solutions; each solution is called a "chromosome." Chromosomes are stored in the computer in binary form. The binary chromosome is converted to decimal values for the purpose of calculations. Calculated values for each chromosome are compared for relative "fitness" as a solution to a set of optimization criteria. A new population is created using three genetic operators' reproduction, mutation and crossover. This population in turn is then evaluated for fitness and the process is repeated until a programmed stopping criterion is reached.

2.4.1 GA characteristics

- 1. Easy to program and understand.
- 2. Domain independent search method.
- 3. Do not get stuck on local optima.
- 4. Support multiobjective optimization.
- 5. Always has an answer, the answer improves with greater computation time.
- 6. Easy to search in a large search space.

Disadvantages

- 1. They are very slow.
- 2. They give better solution but not the absolute best solution.

GAs have been applied in many applications and research areas such as numerical problems, knapsack problems, traveling salesman problem and sequence scheduling, euler path, finding shape of protein molecules, designing neural networks, and functions of creating images. GAs has been successfully applied for optimal design of shell and tube heat exchangers [22]. A case study has been made for the examination of performance of GAs. It concludes that combinatorial algorithms such as GAs provide significant improvement in the optimal design compared to other traditional designs. The GA application for determining the global minimum heat exchanger cost is significantly faster and has an advantage over other methods in obtaining multiple solutions of same quality, which provide flexibility to the designer [22].

2.5 Incorporation of nanofiber in microfiber

Nanofibers are small sized fibers of diameters less than a micron. They have large surface area per unit mass. Nanofibers can be formed in low density, large surface area to mass, highly porous structures that are appropriate for various industrial, consumer, and military filtration applications [23]. Polymeric nanofibers have been used in commercial air filtration over the last twenty years. Nanofiber filter media have enabled new levels of filtration performance in several diverse applications with broad range of environments and contaminants [24]. These filter media improve filter life and dust holding capacity. Nanofibers are used in high efficiency filter media, protective clothing material, drug release membranes, nanotube materials, chemical catalytic materials, bio-transplant materials, and in hydrogen storage tank for fuel cell, etc. Polymeric nanofibers can be produced using the electrospinning process [27].

Electrospinning

Electrospinning is a process to make nanofibers with fiber diameters in the range of about 10 nm to several hundred nanometers from polymer solution through electrostatic forces. As shown in Figure 2.3, when a voltage is applied to the polymer solution, the charged solution overcomes the surface tension and form fibers due to electrostatic repulsion forces.



Figure 2.3 Schematic showing electrospinning set up

Hajra et.al showed that addition of nanofibers to microfibers filter medium significantly improves capture efficiency of sub micron particles [25]. Overall filter performance can be improved by adding nanofibers to the microfiber filter media for the most penetrating aerosol particle sizes [26]. Smaller fibers leads to higher pressure drop, but interception and diffusion efficiencies increases at a faster rate than the pressure drop. The nanofibers contribute to the pressure drop as well as to the capture efficiency. Thus in capturing of submicron and micron particles, better filter efficiency can be achieved at the same pressure drop [27]. Therefore due to dependence of filter efficiency and pressure drop on fiber sizes, small fiber sizes of 0.2 to 0.3 micron diameter are highly recommended for filtration application. Filter media can be designed to optimize the particle removal without creating excessive pressure drop.

CHAPTER III

MODELING AND RESULTS

The filter is modeled where an aerosol is assumed to penetrate the media via depth filtration. Some assumptions have to be considered to simplify the model. The theoretical equations are complicated and have many more unknowns than equations. To make the set of equations more tractable for the optimization calculations to be completed within a reasonable timeframe, a number of assumptions are applied.

3.1 Assumptions

- 1. The fibers in the filter medium are rigid and stationary
- 2. The medium is incompressible.
- 3. The process is isothermal.
- 4. The flow is constant and one-dimensional
- 5. The solid particles are captured on the fibers (not on other particles).
- 6. The filter is clean (no accumulated particles).
- In the momentum balance the pressure drop and drag terms are assumed to dominate, the other mechanisms are neglected.

3.2 Particle Capture Mechanism

Fibrous filters remove submicron and micron particles through different mechanisms which include diffusional deposition, direct interception, inertial impaction and gravitational deposition.

1. Diffusional deposition

In this mechanism the particles in the range of 0.001 to 0.2 μ m range collide with fibers and are captured due to random brownian motion. This random motion occurs when particles collide with gas molecules, thereby moving completely independent of the bulk air stream as gaseous molecules in flowing air. The particles adhere to the fiber surface via intermolecular forces. Diffusion efficiency is a function of the flow field and the Peclet number P_e.

$$Pe = \frac{d_i V}{D}$$
 3.1

Where, d_i is fiber diameter, V is fluid velocity and D is Particle diffusion coefficient



Figure 3.1 Schematic of Diffusion Deposition

2. Direct Interception

The particles in the range of 0.1 to 1 μ m size are captured due to this mechanism. Interception occurs when the fiber diameter is smaller that the particle diameter, the particle is brought within one particle radius of the fiber as it follows the flow streamline and captured. Interception efficiency is a function of the flow field and the size ratio N_R.

$$N_R = \frac{d_P}{d_i}$$
 3.2

where d_p is the particle diameter.



Figure 3.2 Schematic of Interception Mechanism

3. Inertial impaction

Particles of size $1\mu m$ and larger are removed by this method. In this the particles are captured due to their mass and they develop momentum to deviate from the air flow stream line when the stream line bends to flow around a fiber. The inertial efficiency is a function of stokes number St. St is defined as

$$St = \frac{\rho_p C d_p^2 V}{18\eta d_i}$$
3.3

Where, ρ_p is particle density, C is Slip correction factor and η is Gas viscosity



Figure 3.3 Schematic of Inertial Impaction mechanism

4. Gravitational deposition

Particles of greater than 10µm size at relatively low velocities can be captured by this mechanism.

$$E_G = \begin{pmatrix} \rho g d_i^2 / \\ / 18 \mu V \end{pmatrix}$$
 3.4

Where, E_G is single fiber capture efficiency due to gravitational deposition, g is acceleration due to gravity, ρ is fluid density, d_i is fiber diameter

3.3 Conservation Equations

Multiphase transport theory has been employed to aid the modeling. Volume averaging theory provides the general transport equations for the aerosol flow through the filter medium [2].

Gas phase:

• Oil Species Balance:

$$\frac{\partial(\varepsilon\rho_A)}{\partial t} + \frac{\partial(\varepsilon\rho_A v_z)}{\partial z} + \underline{\nabla} \cdot \varepsilon \underline{j}_A - \varepsilon r_A + E_A + G_A + I_A = 0$$
3.5

• Momentum Balance (z component):

$$\frac{\partial(\varepsilon\rho\underline{\nu})}{\partial t} + \nabla \cdot (\varepsilon\rho\underline{\nu}\underline{\nu}) + \varepsilon\underline{\nabla}P + \underline{\nabla} \cdot (\varepsilon\underline{\tau}) + \underline{F} - \varepsilon\rho\underline{g} + (\underline{E} + \underline{G}) = 0$$
 3.6

Here, *I* is the interphase mass transfer, *E* represent convective transport across the interphase between the phases, *G* is generation at the interface due to heterogeneous reaction, $\underline{\tau}$ is the shear stress, r_A rate of mass generation due to homogenous reaction, \underline{j}_A is the species mass flux vector. The gas phase species balance is used to determine the outlet particle concentration. The gas phase momentum balance is used to determine the pressure drop across the media. With the above stated assumptions the balances reduce to:

Oil Species Balance

$$\frac{d(\varepsilon w \rho v_z)}{dz} + I_A = 0 \tag{3.7}$$

Here ε is the void volume fraction (porosity) of the filter, w is the particle mass fraction in the gas, ρ is the gas phase density, and v_z is the gas phase velocity in the z direction. The species balance is solved by introducing a constitutive equation for the interphase mass transfer term I_A related to the filter coefficient, α , by

$$I_{A} = \alpha w \rho \varepsilon v_{z}$$
 3.8

A relation for calculating the filter coefficient, α , as it is dependent on the fiber size and amount of each fiber is derived in a later section.

Momentum Balance (z component)

$$\varepsilon \frac{dP}{dz} + F_z = 0 \tag{3.9}$$

Here P is the local pressure in the gas phase. To solve the momentum balance a constitutive relation for the drag force term, F_z must be introduced.

3.3.1 Calculation of outlet concentration

To determine the outlet concentration Eq.3.7 is rearranged to obtain

$$\frac{dw}{dz} = \frac{-I_A}{\varepsilon \rho v_z}$$
3.10

Substituting 3.8 into 3.10 and canceling terms gives

$$\frac{dw}{dz} = -\alpha w \tag{3.11}$$

On integrating Eq 3.11 from 0 to z gives a general expression for the concentration of particles in the gas stream as a function of depth within the filter.

$$w(z) = w_{IN} \exp(-\alpha z)$$
 3.12

where w_{IN} is the inlet mass fraction. The outlet mass fraction in the gas stream is obtained from Eq.3.11 as

$$w_{OUT} = w_{IN} \exp(-\alpha L)$$
 3.13

Filter Coefficient (α)

The filter coefficient α is related to the single fiber capture efficiency of fibers of diameters d_i as given by

$$\alpha = \sum_{i=1}^{n} E_i \alpha_i \qquad 3.14$$

where E_i is the overall single fiber efficiency taking into account mechanisms of direct interception, inertial impaction, Brownian diffusion, and gravity, given by Brown [2]. The overall efficiency E_i is defined as

$$(1 - E_i) = (1 - E_{Ri})(1 - E_{Ii})(1 - E_{Di})(1 - E_{Gi})$$
3.15

where $(1 - E_{Ri})$ is the fraction of particles that escape from capture by direct interception. Similarly the fraction of particles escaping from the other mechanisms are given inertial impaction $(1 - E_{Ii})$, diffusion $(1 - E_{Di})$, and gravity $(1 - E_{Gi})$. Correlations for these mechanisms are available in [2] and [7].

$$E_{Ri} = \frac{1}{2Ku} \left\{ 2(1+N_R) \ln(1+N_R) - (1+N_R)(1-\varepsilon_i) + (1+N_R)^{-1} \left(1-\frac{\varepsilon_i}{2}\right) - \frac{\varepsilon_i}{2} (1+N_R)^3 \right\}$$
3.16

where ε_i is the volume fraction of fibers of diameter d_i in the medium. The correlations account for slip-flow effects when the Knudsen numbers are greater than 0.01.

$$E_{Ri} = \frac{\left\{ \left(1 + N_R\right)^{-1} - \left(1 + N_R\right) + 2\left(1 + 1.996Kn\right)\left(1 + N_R\right)\ln(1 + N_R)\right\}}{\left(2\left(-0.75 - 0.5\ln(\varepsilon_i)\right) + 1.996Kn\left(-.0.5 - \ln(\varepsilon_i)\right)\right)}$$
3.17

The Knudsen number is defined as

$$K_n = \frac{2\lambda}{d_i}$$
 3.18

where λ is the mean free path of the molecules in the gas stream.

$$Ku = \left(-\frac{1}{2}\ln(\varepsilon_i) - 0.75 + \varepsilon_i - \frac{\varepsilon_i^2}{4}\right)$$
 3.19

The single fiber efficiency for capture by diffusional deposition is given as [2]

$$E_{D_i} = 2.27 P e^{-2/3} \left(1 + 0.39 K n P e^{-1/3} \zeta^{'-1/3} \right)$$
 3.20

In reality, the multiple mechanisms act together for capture of sub-micronic particles along with the aerodynamic slip affect on direct interception and brownian diffusion. R.C. Brown has given the slip affect as [2],

$$E_{RD}' = 1.24\zeta'^{-0.5} P e^{-0.5} N_R^{2/3}$$
 3.21

Overall single fiber efficiency, E_{RD} is given by,

$$E_{RD} = E_R + E_D + E'_{RD}$$

$$3.22$$

The single fiber efficiency is defined as the ratio of the number of particles actually removed relative the number that would be removed if particle capture was proportional to the projected area of the fibers. The projected area is used to define α_i as

$$\alpha_i = \frac{4\varepsilon_i}{\pi d_i} \tag{3.23}$$

3.3.2 Calculation of Drag Force and Pressure drop

The total force acting on all fibers, F_{TOT}, is given by

$$F_{TOT} = A \Delta P$$
 3.24

We define the force per unit length of fiber as *f*. For a filter of multiple fiber diameters the pressure drop is related to the force per unit length by

$$A\Delta P = \sum_{i=1}^{n} L_i f_i$$
 3.25

where L_i is the total length of fibers of diameter d_i within the filter.

Integration of Eq.3.9, assuming uniform properties over the filter thickness, the pressure drop is related to the drag force by

$$\Delta P = \frac{F_z L}{\varepsilon}$$
 3.26

where F_z is the total drag force and L is the thickness of media.

Combining Equations 3.25 and 3.26 we get the expression for the drag force to be

$$F_Z = \frac{\varepsilon \sum L_i f_i}{AL}$$
 3.27

The volume fraction of the filter occupied by the fibers of diameter d_i is defined as

$$\varepsilon_i = \frac{V_i}{AL} \tag{3.28}$$

where V_i is the fiber volume, A is the filter inlet area and L is the filter depth. The volume occupied by the fibers of diameter d_i is given by

$$V_i = \frac{\pi d_i^2 L_i}{4} \tag{3.29}$$

Hence, combining Eqs.3.28 and 3.29 the length of the ith fiber is given by

$$L_i = \frac{4AL\varepsilon_i}{\pi d_i^2}$$
 3.30

Substituting Equation 3.30 in 3.27, we get the relation for the local drag force to be

$$F_{Z} = \frac{4\varepsilon}{\pi} \sum \left(\frac{\varepsilon_{i}}{d_{i}^{2}} f_{i}\right)$$
 3.31

If the medium has only one fiber size, then through use of Eqs.3.31 and 3.26 existing correlations relating pressure drop to flow rate can be used to determine expressions for the functions f_i . For example, for fibers of diameters in the slip flow range $0.01 < K_n < 0.25$, given by Brown [2] the pressure drop relation is

$$\Delta P = \frac{16\mu\varepsilon\upsilon_{z}(1+1.996Kn)\pi d_{i}^{2}\varepsilon_{i}}{d_{i}^{2}\left[-0.5\ln(\varepsilon_{i})-0.75+\varepsilon_{i}-\frac{\varepsilon_{i}^{2}}{4}+1.996Kn(-0.5\ln(\varepsilon_{i})-.025+\frac{\varepsilon_{i}^{2}}{4}\right]} 3.32$$

and the expression for f_i is

$$f_{i} = \frac{4\mu\pi\varepsilon\upsilon_{Z}(1+1.996Kn)}{\left[-0.5\ln(\varepsilon_{i}) - 0.75 + \varepsilon_{i} - \frac{\varepsilon_{i}^{2}}{4} + 1.996Kn(-0.5\ln(\varepsilon_{i}) - .025 + \frac{\varepsilon_{i}^{2}}{4}\right]} \quad 3.33$$

Other correlations are used for other ranges of Knudsen number.
The Quality Factor, QF, is a measure of the particle capture efficiency relative to the energy (*ie.*, pressure drop) required for the separation. The QF is defined by the expression [2]

$$QF = \frac{-\ln\left(\frac{w_{out}}{w_{in}}\right)}{\Delta p}$$
 3.34

Combining Eqs. 3.13, 3.26, 3.31, and 3.34 gives the working equation for calculating the QF,

$$QF = \frac{\alpha}{\frac{4}{\pi} \sum \left(\frac{\varepsilon_i}{d_i^2} f_i\right)}$$
 3.35

For comparison between filter media we define the relative quality factor, RQF, as

$$RQF = \frac{QF}{QF_{CTRL}}$$
3.36

where the QF_{CTRL} is the QF for a control filter medium against which other media area compared.

3.4 Model Calculations

The model is easily programmed into a spreadsheet or in programming software such as C or FORTRAN. As an example, the filter is modeled at room temperature, atmospheric pressure, with air face velocity of 2.1 m/s. The filter is disk shaped 1 cm thick and 6 cm in diameter. The filter is challenged with a concentration of 500 ppm mass fraction of 150 nm spherical particles. The filter is made of 3 grams of 2 micron diameter microfibers having a density of 2500 kg/m³. Varying amounts of nanofibers of different diameters are added to the filter. The filter porosity is determined from the volumes of the fibers present in the filter.

The amount of nanofibers in the filter is calculated as the ratio of the external surface area of the nanofibers divided by the external surface area of the microfibers in the filter medium. An area ratio of zero means no nanofibers are present in the filter. The QF for filter media with zero nanofibers are used as the control value, QF_{CTRL}

Figure 3.4 shows the RQF curves for three different nanofiber sizes. The RQF increases rapidly with small additions of nanofiber, reaches a maximum at around an area ratio of about 1 or 2, and then declines at a slower rate. The rapid increase in RQF is due to the significant increase in surface area available for capture of particles. The RQF passes through a maximum and declines because as more nanofiber is added to the filter the pressure drop increases more rapidly than the capture efficiency.



Figure 3.4 Relative Quality Factor for different nanofiber sizes and area ratios for filters of 3 micron microfibers and challenged with 150 nm particles [16]

Sensitivity analysis of the filter

Sensitivity analysis for the filter is conducted to study the variation in quality factor. The base case is taken at temperature of 21^oC, 20 Psi pressure, face velocity of 2.1 m/sec, particle diameter of 150nm, 2 micron microfiber diameter, 200nm nanofiber diameter, 1 cm thickness of media, 3gms of microfiber and area ratio of nanofiber to microfiber as 0.1. The quality factor calculated for the base case is 0.135 (1/Kpa). Effect of diameter of nanofiber, diameter of microfiber, particle diameter, thickness of media, area ratio, mass of microfiber, temperature and face velocity on quality factor is shown in Figure 3.5. Figure 3.5 shows that diameter of nanofiber, particle diameter and face velocity have dominant effects on the quality factor. The variations in quality factor due to fiber amounts, fiber sizes and other design parameters suggest that a computer program

may be written to determine optimum design values where the filter has maximum performance.



Figure 3.5 Effect of parameters on quality factor

CHAPTER IV

COMPUTER PROGRAM

4.1 Approach

To optimize the filter design we apply a Genetic Algorithm (GA). GAs are robust in selecting optimum size and amounts of nanofiber and microfiber and other design parameters for composite filter media. GAs are used in search and optimization, such as finding the maximum of a function over some domain space [28]. A flow chart describing the major steps in applying the GA to filter design is shown in Figure 4.1.



Figure 4.1 Flowchart for applying a Genetic Algorithm to optimize filter design

A random number generator is used to initialize a population of solutions. Each solution consists of the values of several variables that are being optimized. In our program, the variables being optimized are the thickness of the filter medium, the diameter of the micro fibers, the diameter of the nanofibers, the area ratio of the nanofibers to microfibers, and the mass of the microfiber (in a 6 cm diameter disk). A range is given for each variable over which the search is conducted. Each solution in the population is evaluated by calculating the QF (fitness function) for that solution.

4.2 Fitness Function

The fitness function links the Genetic Algorithm to the problem to be solved. The optimization problem can be used to maximize or minimize a function. Our program is based on maximizing the function "Quality Factor" for efficient filter performance. The best fit solution in the final generation is the one that maximizes the quality factor. The program will calculate quality factor for each set of solutions until a stopping criterion is reached. The fitness function evaluates each solution to decide whether it will contribute to the next generation of solutions. Then, through operations analogous to gene transfer in sexual reproduction, the algorithm creates a new population of candidate solutions.

4.3 Convergence

Convergence is the final problem to stop the execution of the algorithm. A stopping criterion is checked to see if it is satisfied. In our program the user specifies the maximum number of populations to be evaluated. When this maximum is reached the program stops. A second stopping criterion is also applied in which the change of the

maximum QF to the number of generations between changes is monitored and if this change rate becomes smaller than a user specified value then the program stops. When the stopping criteria is not satisfied the program proceeds to generate a new population. Convergence of less than 10^{-8} is recommended for a better solution. Each new population is generated by three genetic operators.

The new population is generated by copying existing solutions into the new population. The number of copies of each solution are weighted to make more copies of the best solutions and fewer copies of the worst solutions. This is analogous to the "survival of the fittest" from evolutionary theory. The solutions are stored in the computer in binary form that makes it possible to apply cross-over in which bits between two parents from the previous generation are exchanged to create a new offspring solution. Also, a small number of the new solutions are randomly selected for mutation, in which one of the bits in the solution is randomly selected and changed from 0 to 1 or 1 to 0. The cross-over and mutation creates solutions in the new population different from the previous population that enables the search to extend to other parts of the solution space.



Figure 4.2 Screenshot of program FiL2RO

4.4 Input and Outputs

Figure 4.2 shows screenshot of the program FiL2RO. The input parameters are operating conditions such as pressure, temperature, air face velocity (inlet velocity of air entering into the filter), diameter of filter media, particle size which needs to be captured and density of microfiber. The ranges for the five physical parameters of filter media namely thickness of media, diameter of microfiber, diameter of nanofiber, area ratio of nanofiber to microfiber, mass of microfiber that needs to be optimized are entered. Finally the genetic algorithm parameters such as population is fixed at 1000, but the number of generations, mutation rate and the convergence value can be set by the user. Depending on the convergence tolerance, the program stops and shows the result. If convergence tolerance is not achieved, the number of generations can be increased and the program can be re-run. A convergence tolerance of less than 10⁻⁸ is recommended to get better solutions.

The output shows the optimum design parameters of filter media with generation at which the program got converged and quality factor. It also calculates the porosity, pressure drop, and permeability of the best medium at program convergence. The generation vs. convergence and quality factor vs. selected design parameters can be plotted after the program has converged.

4.5 Features of program

- 1. Interactive presentation of data to enable user input and interpretation of the calculated data.
- 2. Warns the user if input data are incorrectly entered or if data are missing.
- 3. Conversion of units according to your choice.
- 4. Output data in graphical and tabular format.
- If the convergence is not achieved it warns the user to increase the iterations or increase the convergence.
- 6. User can view input parameters and graphical interpretation of final result.
- 7. Results can be saved into a file to be viewed later.
- 8. All data required for filter design are shown.

Limitations

- 1. Particles are spherical in shape.
- 2. Surface properties are not considered.
- 3. Uniform distribution of fibers in media.
- 4. Gas phase is incompressible (small pressure drop)
- 5. Steady state momentum (after loading)

- 6. GA is iterative in nature hence time consuming.
- Diffusion and interception mechanism are dominant only in sub micron sized particles.

4.6 Results

The computer program is written in Fortran and Visual basic to allow the user to input operating conditions such as the size of the particle to be captured, gas temperature, flow rate, etc. It is not practical to try to test each of these conditions to report on the optimum design parameters for the filters. However we have made several general observations that we report here.

Diameter of particle		150nm	500nm	1000nm
Parameters	Search Range	Optimum	Optimum	Optimum
Thickness of media (m)	0.01-0.02	0.014	0.0172	0.013
Diameter of microfiber (microns)	1-10	1.03	1.07	1.02
Diameter of nanofiber (nm)	10 -1000	10	10	10
Area ratio	0.1-10	9.76	9.9	9.85
Mass of microfiber (kg)	0.002-0.01	0.00252	0.00275	0.0022
Convergence		3.40E-09	3.64E-09	1.94E-09
Quality factor (per Kpa)		5.26E-03	1.78E-02	3.65E-02
Porosity		0.972	0.975	0.973
Pressure drop (Kpa)		1.45E+04	1.55E+04	1.29E+04
Permeability (m ²)		3.94E-11	4.50E-11	3.96E-11
Generation		35256	137865	134957

Table 4.1 Results from software program for several particle diameters

Diameter of particle		150nm	500nm	1000nm
Parameters	Search Range	Optimum	Optimum	Optimum
Thickness of media (m)	0.01-0.05	0.048	0.0491	0.0488
Diameter of microfiber (microns)	1-10	9.98	9.73	9.99
Diameter of nanofiber (nm)	200-1000	200	200	200.04
Area ratio	0.1-10	1.81	1.91	1.9
Mass of microfiber (kg)	0.001-0.008	0.001	0.001	0.001
Convergence		4.97E-10	2.82E-09	4.41E-11
Quality factor (per Kpa)		4.40E-04	1.69E-03	3.97E-03
Porosity		0.997	0.997	0.997
Pressure drop (Kpa)		2.33E+01	2.54E+01	2.44E+01
Permeability (m ²)		8.50E-08	7.82E-08	8.10E-08
Generation		34554	18296	190420

Table 4.2 Results from software program with different parameter ranges

Table 4.3 Results from software program showing the optimum value for area ratio

Parameters	Search Range	Optimum
Thickness of media (m)	0.01	0.01
Diameter of microfiber (microns)	2	2
Diameter of nanofiber (nm)	200-1000	200
Area ratio	0.1-10	2.02
Mass of microfiber (kg)	0.003	0.001
Convergence		7.56E-9
Quality factor (per Pa)		3.21E-04
porosity		0.949
Pressure drop (Kpa)		9.55E+02
Permeability (m2)		4.24E-10

Tables 4.1, 4.2 and 4.3 show sample results from the software program. The calculations assume conditions of room temperature, atmospheric pressure, with air face velocity of 2.13 m/sec, the diameter of filter disk is 6cm, and the density of the micro fibers is 2500 kg/m3. The program was run for three different particle sizes of 150nm, 500nm, 1000nm. The two tables compare results for different search ranges for the media thickness, nanofiber diameter, and mass of microfiber in the filters. The tables show the characteristics of media and number of iterations the program takes for the convergence criterion to reach less than 10^{-8} . The program took about 30 minutes to give optimal solutions.

We observe from the data in the tables that when we take minimum value for nanofiber diameter as 10nm or less that the optimum values for thickness of media, and mass of microfiber are between the extremes specified in the search range limits, the microfiber diameter goes to the minimum value, and the external surface area ratio of nanofiber to microfiber goes to the maximum value. The pressure drop for this filter design is high. In the Table 4.1 when we take minimum value for nanofiber diameter as 200 the optimum values for thickness of media and the diameter of microfiber goes to maximum in the search range limit, the optimum values for nanofiber diameter and the mass of microfiber go to the minimum in the range limits, and the surface area ratio of nanofiber to microfiber falls between the range limits. For this filter design the pressure drop is lower compared to data obtained in Table 4.2 and the quality factor is lower when compared to data in Table 4.1. Table 4.3 shows that optimum value for area ratio is 2.02 for 150nm particle diameter for a range of 0.1 to 10 and diameter of nanofiber as 200nm for a range of 200-1000nm, fixing the other variables.



Figure 4.3 Thickness of media vs. Quality Factor and Pressure drop

Figure 4.3 shows the variation of quality factor and pressure drop with thickness of media. The optimum solution for thickness of media is calculated from the program. The data plotted in this figure are for microfiber diameters of 2 microns, mass of microfiber is 0.002 kg and the area ratio of nanofiber to microfiber is 1. The range for the thickness of media is 0.01-0.05 m and the diameter range of the nanofiber is 10-1000 nm. The optimal solution for the thickness of media is 2.79 cm and the optimum nanofiber diameter is 10 nm.



Figure 4.4 Mass of Microfiber vs. Quality Factor and Pressure drop

Figure 4.4 shows the variation of quality factor and pressure drop with mass of microfiber. The optimum mass of microfiber in a 6 cm diameter disk filter 0.02 m thick is plotted in this figure. In the program calculations the diameter of microfiber is 2 microns and the area ratio of nanofiber to microfiber is fixed at 5. The search range of mass of microfiber is 0.001-0.008 kg and search range for the diameter of nanofibers is 10-1000 nm. The optimal mass of microfiber obtained is 0.003 kg and the optimum nanofiber diameter is 10 nm.

We can conclude from the data in Tables 4.1, 4.2 and 4.3 that smaller fibers contribute to higher pressure drop but also contribute to greater capture efficiency. The quality factor increases as long as the capture efficiency increases faster than the pressure drop. The plots in Figures 4.3 and 4.4 show that there are optimum values for thickness

of media and mass of microfibers. Sometimes the optimums occur within the specified search range and sometimes the optimum occurs at either the upper or lower limits of the search ranges. When the optimum occurs at the limits this suggests that the search ranges should be expanded, but that that will be a topic for further study.

Overall, there are observable trends in the optimum design parameters. However, because there are so many design parameters and it is not easy ways to represent all of the optimum design conditions such as on a single plot or chart. A computer search code such as described here is a valuable tool for helping design engineers to determine optimum designs.

CHAPTER V

FILTER MEDIA PREPARATION AND CHARACTERIZATION

5.1 Filter Media Preparation Slurry preparation

A measured quantity of glass fibers having diameters of 2 microns are dispersed in water in a slurry tank. About 3ml of carboset 560 binder is added to bind the fibers together. Carboset 560 (supplied by B.F.goodrich) is an acrylic polymer dispersed in water; milky white in appearance. Acid is added to maintain pH in the range of 2.5-3.0 for uniform mixing of fiber. The solution is stirred for 24 hrs. Then the slurry is vacuum molded to form filters of 6cm diameter. There are several methods for mixing nanofiber and microfiber to make filter media of mixed fiber. The polymer solution can be directly electrospun into the prepared microfiber slurry. After a certain amount of nanofiber is collected, the slurry is continuously mixed with air bubbles. Another method of adding nanofiber is to chop up the required amount of nanofiber and then make slurry of mixed fiber of microfiber and chopped nanofiber and vacuum molded to the make the filter medium. Microfiber and nanofiber composition are B-glass fiber of diameter 2 microns and nylon nanofiber of diameter 200nm which is electrospun at the rate of 2µl/min and voltage of 20KV. Figure 5.1 shows the SEM image of electrospun nylon nanofiber.

Filter media containing different amounts of nylon nanofiber and 3 gms of microfiber are prepared using vacuum molding and tested using the coalescence filtration

apparatus. The amount of nanofibers added to the filter medium is based on the ratio of surface area of the nanofibers to microfibers, A_{nf}/A_{mf} . Filters are prepared with the $A_{nf}/A_{mf} = 0.0, 0.05, 0.4, 0.8 1.2, 3.6$. The amount of nanofibers is varied depending on the desired value of A_{nf}/A_{mf} .



Figure 5.1 SEM image of electrospun nylon nanofiber on a 2 micron glass fiber



Figure 5.2 Vacuum mold assembly

The vacuum mold consists of collecting tank and a vacuum pump which is capable of generating pressure of about 100mm to 500mm mercury. The prepared slurry is poured into the mixing tank. The mixing tank is connected to the mold which is connected to a vacuum hose. The filter cake is formed over the steel mesh screen in the mold. With vacuum pressure all the acidic solution is collected in the tank and discarded and a cylindrical shaped filter of 6cm diameter is formed. The wet filter media is removed from the mold and heated in an oven at about 120-150^oC to ensure proper curing of the binder.

5.2 Filter Media Characterization

Fiber parameters, such as fiber type, fiber fineness, cross-sectional shape, and filter parameters, such as mass per unit area, fiber packing fraction, thickness, and surface characteristics, play a major part in determining the filter media structure and related properties, in particular pore size distribution, and air permeability. Porosity, permeability and hardness will provide the information how the media will perform.

Porosity

Porosity of Filter media is measured using pycnometer shown in Figure 5.3. Porosity is void fraction present in the filter medium. Porosity of fibrous filters consisting of a mat of fine fibers arranged in such a way that most are perpendicular to the direction of air flow have the porosity from 70% to more than 99%. Flow rate is directly proportional to the porosity of the media; higher porosity means higher flow rate, for a given pore size and thickness of filter medium.



Figure 5.3 Pycnometer set up in the laboratory

Frazier permeability test

Permeability is the ability of medium to allow the passage of liquid though the pores of medium. The permeability of a medium is defined by Darcy's equation describing flow through a porous layer. Higher the permeability lesser will be the resistance to airflow. Permeability is measured using the Frazier test in Figure 5.4.

$$K = \frac{Q}{A} \mu \frac{L}{\Delta P}$$
 5.1

where,

K=Permeability coefficient

 ΔP = Pressure drop

L=Thickness of media

Q=Volumetric flow rate

 μ = viscosity

A=Area



Figure 5.4 Frazier's Permeability set up in the laboratory Hardness

A durometer is used to measure the hardness of the filter medium defined as the material's resistance to permanent deformation.

Table 5.1 shows the characteristics of filter media for different amount of nanofibers. Nanofibers increase the volume fraction of the fibers and reduce the void spaces thus decreasing the porosity. Nanofibers have tighter pore structure which reduces the permeability of the media, but have lower hardness.

Area ratio	Porosity	Permeability (k *10^11, m ²)	Hardness
0	0.9	6.3	25
0.38	0.85	4.2	23
0.78	0.84	3.29	22
1.17	0.81	2.8	18
2.02	0.8	2.5	16
3.6	0.78	1.03	14

Table 5.1 Average porosity, permeability and hardness of the filters

CHAPTER VI

EXPERIMENTAL RESULTS AND DISCUSSIONS

6.1 Coalescence Filtration

A coalescence filtration apparatus shown in Figure 6.1 is used to determine the pressure drop and efficiency of a media. The main components of the coalescence filtration apparatus are: pressurized air supply, Laskin nozzle for generating oil droplets, filter holder, and Scanning Mobility Particle Sizer (not shown in figure).



Figure 6.1 Coalescence Filtration set up in the laboratory

The cylindrical test media of 6cm diameter and thickness of 1 cm is inserted in a filter holder and the steel mesh is placed to give support to the filter at higher pressure drops. The upstream section comprises various elements to generate the aerosol. The Laskin nozzle is used to generate oil droplets in order to challenge the filter medium and the filtered compressed air at a flow rate of $0.0035 \text{ m}^3/\text{sec}$. The oil used in the Laskin nozzle is propylene glycol. Moisture in the compressed air stream is removed using a dryer. The exit stream from the dryer splits into two streams, one stream passes into the Laskin nozzle for generating oil droplets under pressure. The other stream passes through a pressure regulator on its way to the filter sample. A pressure regulator is used to attain the desired pressure drop across the Laskin nozzle. The exit air stream from Laskin nozzle carries oil droplets in the form of an aerosol. A differential pressure transducer (Omega PX 7771) is used to measure the pressure at the upstream and downstream. A photometer (Air Techniques TDA-2G) is used to verify the steady state. The Photometer is used to measure the concentration, once it is calibrated. A Scanning Mobility Particle Sizer, SMPS (TSI instruments, Model 3080) is used to measure the particle size distribution

The aerosol was sampled upstream and downstream of the media. The particle size distribution was measured by SMPS. The data from SMPS are analyzed for measuring the inlet and outlet concentration of the aerosol.

A High Efficiency Particulate Air, HEPA filter at the downstream captures the oil and prevents the oil from entering into the rotameter (Omega, series FL 86). The flow rate to the rotameter is kept constant for all filter experiments.

6.2 Results and Conclusion

Performance of filters from coalescence experiments:

Filters with various area ratio of nanofiber to microfiber were analyzed. The experiment runs until a steady state is reached in pressure drop and outlet concentration. Pressure drop, saturation and quality factor at steady state are compared. Quality factor is calculated taking the inlet and outlet concentration data which are obtained from SMPS and pressure drop using pressure transducer at steady state. Figures 6.2 and 6.3 show quality factors from experiments and from the model as a function of the area ratio analogous to Figure 3.4. The quality factor increases with addition of nanofibers and reaches an optimum value and then decreases.

Figure 6.4 shows pressure drop trend with addition of nanofiber.. The pressure drop increases on adding nanofibers which makes quality factor to decrease. Figure 6.5 shows the SMPS data for particle size distribution. The plot shows the diameter of particle versus droplet count per cubic centimeter of air measured for outlet and inlet concentration for area ratio of 3.6 (0.45 gm of nanofiber).



Figure 6.2 Experimental quality factor versus A_{nf}/A_{mf}



Figure 6.3 Quality factor versus $A_{nf}\!/A_{mf}$ from modeling



Figure 6.4 Pressure Drop versus Anf/Amf



Figure 6.5 Concentration profile versus particle size

Comparison of model with experiment

Table 6.1 shows a set of experimental and computer data. An experiment was conducted on filter media with specific properties including an area ratio of 0.78. The same filter characteristics were entered into the computer program to calculate the quality factor. Table 6.2 shows the QF from experiments as 0.24 and QF from computer program as 0.297

Table 6.2 shows the optimum quality factor from experiments and the computer program. In the computer program the search range is given for diameter of nanofiber and area ratio and the optimum area ratio comes out to be 2.02 which is shown in Table 4.3. Figure 6.2 shows the optimum QF value as 0.27 KPa⁻¹, whereas the optimum QF calculated by FiL2RO is 0.321 KPa⁻¹. These experiments were conducted on filter media having properties as close to the predicted properties as could be constructed in our laboratory using the vacuum molding process. This shows the predicted optimum filter design is reasonably close to the experimental optimum.

The difference in the values between the experiments and the computer calculations may be due to certain assumptions taken in modeling which cannot be controlled during experiments. The fiber size and particle size are not uniform during experiments. Hence the averages of three sets for experiments are reported in Table 6.1 and Table 6.2 for comparison with the computed results. However, some experimental conditions are not accounted for in the computer model. The real filter media have binder, which can account for part of the lower porosity (fiber structure and packing also affects the porosity). The model does not account for liquid saturation, which further reduces the available space for gas flow. The computer model results do not exactly match the

experimental results but the results are of the same order of magnitude and show similar trends within about 25% error.

Parameters	Experimental data	Computer Program
Thickness of media (m)	0.01±0.009	0.01
Diameter of microfiber (microns)	2±3	2
Diameter of nanofiber (nm)	200±150	200
Area ratio	0.78	0.78
Mass of microfiber (kg)	0.003	0.003
Porosity	0.84±0.01	0.95
Saturation	0.30±0.02	0
Quality factor (per KPa)	0.24±0.008	0.297

Table 6.1 Comparison of quality factor from experiment and the computer program

Table 6.2 Comparison of quality factor from experiment and the optimum

Parameters	Experimental data	Computer Program
Thickness of media (m)	0.0098±0.001	0.01
Diameter of microfiber (microns)	2±3	2
Diameter of nanofiber (nm)	200±150	200
Area ratio	2.01	2.02
Mass of microfiber (kg)	0.003	0.003
Porosity	0.80±0.02	0.95
Saturation	0.35±0.01	0
Quality factor (per KPa)	0.27±0.01	0.321

from the FIL2RO computer program

In the coalescence filtration, saturation across the filter is estimated and that saturation value is incorporated in the model using the volume averaging equations.

Saturation across the filter is estimated using the following equation [29]

$$Sa = \frac{\left(Mass_{final} - Mass_{initial}\right)}{V_{cake}(1 - \varepsilon_i)\rho_{oil}}$$

$$6.1$$

Mass_{initial} - Mass of the filter before experiment.

Mass final -Mass of the filter after experiment.

 V_{cake} - Volume of the filter.

 ρ_{oil} - Density of oil, i.e., polypropylene glycol = 983 kg/m³

In our modeling we have assumed as clean filter which means that saturation is 0. The range of saturation varied from 0.20 to 0.47 during the coalescence filter experiments. The filter with more amount of nanofiber has higher saturation. At surface area ratios greater than 2 the pressure drop increases faster than the capture efficiency and decreases the QF.

After running a few experiments; the results are encouraging and suggest that the error is reasonable. However a more extensive validation is needed in future work.

CHAPTER VII

CONCLUSIONS AND FUTURE WORK

7.1 Conclusions

This work has 8 objectives. The results for each objective are summarized here.

1. Develop a computational model to predict filter performance for mixed fiber media for depth filtration.

I developed a model using volume averaged continuum equations and multiphase transport theory taking into accounts all the assumptions (Section 3.3). The model calculates single fiber efficiency, pressure drop and the quality factor of the filter media for mixed fiber media. The model shows that quality factor depends on fiber size, fiber quantities and other design parameters of media (Figure 3.5).

2. Selection of design parameters of filter media for optimization.

The basic requirement of filter media is high efficiency and low pressure drop. The computer model finds the best value of five physical parameters thickness of media, diameter of microfiber, diameter of nanofiber, area ratio of naofiber to microfiber and mass of microfiber that optimizes capture efficiency and pressure drop. 3. Develop a software program to find optimum parameter values of mixed fiber filter media design using the Genetic Algorithm search technique.

I developed a computer program FiL2RO that determines optimum design parameter values of the five physical parameters listed in 2. Genetic Algorithm coding and all the modeling equations are written in FORTRAN (Appendix A). The Visual Basic is used for user interface so that the user can input parameters and visualize and interpret the results (Figure 4.2). GA is explained in detail in chapter 4.

4. Selection of fitness function and convergence criterion.

I have chosen Quality Factor as fitness function (Section 4.2). Performance of filter is quantified by Quality factor. Higher the quality factor, the better the filter performs. A convergence criterion is based on maximum number of population and slope of the threshold value of maximum quality factor to the number of generation (Section 4.3).

- Interpret and analyze the results from the software program.
 The program results are shown in chapter 4. The FiL2RO program calculates the optimal solution based on a given range for the five parameters.
- 6. Construct and test filters with varying amounts of nanofibers in glass fiber media. I prepared filters using different amount of nanofiber and the filter media were tested using coalescence experiments to find quality factor and pressure drop. The optimum performances of filters were obtained for surface area ratio of about 2 (Figure 6.2).

- Compare model calculations with experimental data (Figures 6.2 and 6.3). Figures
 6.2 and 6.3 show similar trend with optimum quality factor at area ratio of 2.
- Compare optimum filter performance with optimization program (Table 6.1).
 Coalescence filtration experiments were done to verify the computer modeling results. The results show about 25% error in quality factor between computer and experiment (Table 6.2)

A computer code has been developed that optimizes filter medium design. This program gives physical properties (fiber diameter, amount of fibers and thickness of media) that are expected to give clean media with optimum performance. This design can be used as the starting basis for filter companies to design media with nanofiber for specific applications.

7.2 Future work

The following are some suggestions for the future work:

1. Add particle size and fiber size distributions to the model to get better agreement between the model and experiments.

2. More thorough validation of model to experiment.

3. Model can be extended for multilayered media.

4. Particle loading or saturation can be incorporated in the model.

5. Refinement of the model limiting assumptions like considering effects of binder which accounts for porosity.

6. Model Unsteady State Coalescence stage.

7. Influence of other filter characteristics like loading on filter life.

NOMENCLATURE

- A Area of filter
- d_i , fiber diameter
- E_i Single fiber efficiency
- F_z Drag force
- F_{TOT} Total force acting on a filter
- f_i Drag force per unit length of fiber of diameter di
- *I* Mass flux of particles captured from gas phase onto fibers
- K_n Knudsen number
- *L* Filter thickness
- L_i Total length of fibers of d_i within elemental volume of the filter medium
- ΔP Pressure drop across filter
- QF Quality Factor
- *RQF* Relative quality factor (QF of the medium/QF of medium of only microfibers)

- v_z Intrinsic gas phase velocity in the z direction
- *w* Mass fraction of particles in the gas phase
- w_{in}, w_{out} Inlet and outlet mass fractions of particles in gas phase
- α Overall Filter Coefficient for the filter medium
- α_i Filter Coefficient based on projected area of fibers
- ε Porosity of the media
- ε_i Volume fraction of the fibers with size i
- λ Mean free path
- μ Viscosity of gas phase
- ρ Gas phase density
- *D* Particle diffusion coefficient
- *E* Convective transport across the interpahse between the phases
- *G* Generation at the interphase due to heterogenous reaction
- *I* Interphase mass transfer term
- *Sa* Saturation across the filter

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APPENDICES

APPENDIX A

FORTRAN PROGRAM

Genetic algorithm code and modeling equations are written in fortran program.

This program is designed to find the optimum design parameters of filter media IMPLICIT REAL (A-H, O-Z) IMPLICIT INTEGER (I-N)

PARAMETER (NPOP=1000, NVAR=5,NBIT=22)

!

! NPOP = population size of each generation
! NVAR = number of variables to be fitted by the GA
! NBIT = number of logic bits that represent each variable
! The parameter statement sets the values for these quantities. These
! quantities cannot be changed when the program is running (such as
! by adding lines to the menu). When changing these parameters they must
! be changed in all subroutines where the parameter statement occurs.

LOGICAL CHROM(NPOP,NVAR*NBIT), OLD(NPOP,NVAR*NBIT) COMMON CHROM,OLD,N(NPOP),G(NPOP),F(NPOP),VAR(NVAR) COMMON VOPT(NVAR),FOPT,NGEN,MGEN,PMUT,RAND,IFITTYPE COMMON PABS,T,VO,D,FMDEN,DP,ZMAX,ZMIN,DMFMAX,DMFMIN,DNFMAX,DNFMI N,ANFAMFMAX, ANFAMFMIN,THICKNESSCHK,FMAX,ANFAMFMIN, FMMASSMAX, FMMASSMIN,THICKNESSCHK,DIAMFCHK,DIANFCHK, ARRATIOCHK,MASSMFCHK

! MAIN	PROGRAM	
	CALL INIT	! Initialize variables
	CALL CALC	
	CALL RESULTS	! Calculate generations
	END	
!		
INITIALIZE VARIABLES		
	SUBROUTINE INIT	
	IMPLICIT REAL (A-H, C)-Z)
	IMPLICIT INTEGER (I-N	(7
	!	
PARAMETER (NPOP=1000,NVAR=5,NBIT=22)		
	!	
	LOGICAL CHROM(NPO	P,NVAR*NBIT), OLD(NPOP,NVAR*NBIT)
	COMMON CHROM, OLI	D,N(NPOP),G(NPOP),F(NPOP),VAR(NVAR)
	COMMON VOPT(NVAR	,FOPT,NGEN,MGEN,PMUT,RAND,IFITTYPE

COMMON PABS,T,VO,D,FMDEN,DP,ZMAX,ZMIN,DMFMAX,DMFMIN,DNFMAX,DNFMI N,ANFAMFMAX, ANFAMFMIN,THICKNESSCHK,FMAX,ANFAMFMIN, FMMASSMAX, FMMASSMIN,THICKNESSCHK,DIAMFCHK,DIANFCHK, ARRATIOCHK,MASSMFCHK !REAL Z,D,PABS,T,VO,FMMASS,FMDEN DIMENSION IVALUE(8) CHARACTER CH1,CH2,CH3

MGEN = 0**! COUNTER TO TRACK TOTAL NUMBER OF GENERATIONS** IFITTYPE = 1! FITNESS TYPE. TYPE = 1: THE LARGER THE FITNESS FUNCTION THE BETTER THE FIT ! ! TYPE = 2: THE SMALLER THE FITNESS FUNCTION THE BETTER THE FIT ١ **! SET GLOBAL FITTNESS VALUE** WRITE(*,*)'INPUT VARIABLES INIT' ! IF(IFITTYPE.EQ.1)THEN FOPT=1.E-10 ELSE FOPT=1.E12 ENDIF ! Randomize the seed generator CALL DATE AND TIME(CH1,CH2,CH3,IVALUE) DO I = 1, IVALUE(8) ! CALL RANDOM NUMBER IN LOOP TO VARY THE STARTING VALUE CALL RANDOM NUMBER(RAND) **ENDDO** 1 **! SET CHROMOSOMES FOR INITIAL POPULATION** DO I=1.NPOP DO L=1,NVAR*NBIT CALL RANDOM NUMBER(RAND) **! RANDOM NUMBER** GENERATOR, RETURNS ! A NUMBER 0<= RAND <= 1 IF(RAND.GT.0.5)THEN CHROM(I,L)=.TRUE. ELSE CHROM(I,L)=.FALSE. **ENDIF** ENDDO **ENDDO** SAVING THE OUTPUT INTO GA.DAT FILE OPEN(UNIT=7,FILE='C:\temp\ga.txt',STATUS='UNKNOWN')

! THIS WILL OPEN AN EXTERNAL FILE SAMPLE.TXT IN WHICH THE USER INPUTS ARE STORED (VARIABLES ARE SAVED INTO TEXT FILE VISUAL BASIC PROGRAM. ! THIS OPEN STATEMENT WILL READ THE VARIABLES AND GOTO LOOP TERMINATES WHEN END OF FILE IS REACHED.

!

!OPENING AN EXTERNAL FILE INPUTVAR.TXT WHERE THE DATA IS STORED FROM VISUAL BASIC FILE

OPEN(UNIT=1,file="c:\vbprograms\inputvar.txt", STATUS="OLD")

READING ALL THE VARIABLES FROM INPUTVAR.TXT

8

READ((1,*,END=12)PABS,T,VO,D,FMDEN,DP,THICKNESSCHK,ZMIN,ZMAX,DIAMFCHK,DMFM IN,DMFMAX,DIANFCHK,DNFMIN,DNFMAX,ARRATIOCHK,ANFAMFMIN,ANFAMFMAX,MASS MFCHK,FMMASSMIN,FMMASSMAX,NGEN,PMUT

GO TO 8

12 PRINT *

!

RETURN END

!

! CALCULATE THE FITNESS OF ALL CHROMOSOMES OVER MULTIPLE GENERATIONS SUBROUTINE CALC IMPLICIT REAL (A-H, O-Z) IMPLICIT INTEGER (I-N)

PARAMETER (NPOP=1000,NVAR=5,NBIT=22)

LOGICAL CHROM(NPOP,NVAR*NBIT), OLD(NPOP,NVAR*NBIT) COMMON CHROM,OLD,N(NPOP),G(NPOP),F(NPOP),VAR(NVAR) COMMON VOPT(NVAR),FOPT,NGEN,MGEN,PMUT,RAND,IFITTYPE COMMON PABS,T,VO,D,FMDEN,DP,ZMAX,ZMIN,DMFMAX,DMFMIN,DNFMAX,DNFMI N,ANFAMFMAX, ANFAMFMIN,THICKNESSCHK,FMAX,ANFAMFMIN, FMMASSMAX, FMMASSMIN,THICKNESSCHK,DIAMFCHK,DIANFCHK, ARRATIOCHK,MASSMFCHK

DIMENSION VMAX(NVAR),VMIN(NVAR) !REAL Z,D,PABS,T,VO,FMMASS,FMDEN

> MOPT=0 RPOP=NPOP **! USE REAL VALUE OF NPOP IN CALCULATIONS** DO K=1,NGEN MGEN=MGEN+1 WRITE(*,*)' GENERATION =',MGEN 1 **! EVALUATE THE FITNESS OF EACH CHROMOSOME** FMAX=00FMIN=1000000000000 ! SET INITIAL FMIN TO SOME ARBITRARY LARGE NUMBER DO I=1,NPOP ! I = INDEX TO EACH CHROMOSOME CALL DECODE(I) **! DECODE PARAMETERS FROM** BINARY TO DECIMAL ! F(I)=FUNC() **! FUNC IS USER DEFINED FUNCTION TO BE** FITTED, F>=0 IF(F(I).GT.FMAX)THEN **! STORE MAX VALUES** IMAX=I FMAX=F(I) 68

DO J=1,NVAR VMAX(J)=VAR(J)

ENDDO ELSE IF(F(I).LT.FMIN)THEN IMIN=I ! STORE MIN VALUES FMIN=F(I) DO J=1,NVAR VMIN(J)=VAR(J)

ENDDO

ENDIF

ENDDO

! ! SAVE BEST STRING TO FILE IF (IFITTYPE.EQ.1)THEN

IF(FMAX.GT.FOPT)THEN !FOPT IS THE OPTIMUM FOR ALL GENERATIONS

CONVRG=(FMAX-FOPT)/FOPT/(MGEN-MOPT) MOPT=MGEN !CONVERGENCE SHOULD GO TOWARDS ZERO (10^-8)

FOPT=FMAX DO J=1.NVAR

VOPT(J)=VMAX(J)

ENDDO

WRITE(7,*)MGEN,CONVRG,FOPT,VOPT

ENDIF

ELSE

IF(FMIN.LT.FOPT)THEN

CONVRG=(FOPT-FMIN)/FOPT/(MGEN-MOPT) MOPT=MGEN FOPT=FMIN DO J=1,NVAR

VOPT(J)=VMIN(J)

ENDDO

WRITE(7,*)MGEN,CONVRG,FOPT,VOPT

ENDIF

ENDIF

1

! DETERMINE THE REPLICATION FRACTIONS FOR THE NEXT GENERATION ! See end of subroutine for definitions of fitness and replication parameters FSUM=0.0 DOD = 0.0

DO I=1,NPOP FSUM=FSUM+F(I)

ENDDO

HSUM=(FSUM-NPOP*FMIN)/(FMAX-FMIN)

DO I=1,NPOP

HI=(F(I)-FMIN)/(FMAX-FMIN)

IF(IFITTYPE.EQ.1)THEN G(I)=HI/HSUM

69

! LARGEST F IS BEST

ELSE

ENDIF

G(I)=(1.0-HI)/(RPOP-HSUM) ! SMALLEST F IS BEST

N(I)=G(I)*NPOP+0.5! CALCULATE THE NUMBER OF REPLICATIONS ! OF THE Ith CHROMOSOME ! ADD 0.5 FOR ROUNDUP **ENDDO** ١ **! FORM THE NEW POPULATION ARRAY ! TEMPORARILY SAVE THE PREVIOUS ARRAY** DO I=1,NPOP DO L=1,NVAR*NBIT OLD(I,L)=CHROM(I,L) **ENDDO ENDDO** ١ ! COPY CHROMOSOME INTO NEW POLULATION BASED ON THE FITNESS ISTOP=0 ISTART=0 DO I=1,NPOP IF(N(I).GT.0.AND.ISTOP.LT.NPOP)THEN ISTART=ISTOP+1 ISTOP=ISTOP+N(I) IF(ISTOP.GT.NPOP)ISTOP=NPOP DO J=ISTART,ISTOP DO L=1,NVAR*NBIT CHROM(J,L)=OLD(I,L)**ENDDO** ENDDO **ENDIF** ENDDO ١ ! CROSSOVER: EXCHANGE CHROMOSOME BITS BETWEEN CHOMOSOMES FOR **! EXPANDED SEARCH SPACE** DO I=1.NPOP ! EACH CHROMOSOME HAS A RANDOM CHANCE OF CROSSING WITH ANOTHER I1=I **! FIRST PARENT** ! CALL RANDOM NUMBER(RAND) **! SECOND PARENT** I2=NPOP*RAND+0.5 IF(I2.LT.1)I2=1 IF(I2.GT.NPOP)I2=NPOP ١ **! RANDOMLY SELECT CROSSING POINT** CALL RANDOM NUMBER(RAND) LC=NVAR*NBIT*RAND+0.5 IF(LC.LT.1)LC=1 IF(LC.GT.NVAR*NBIT)LC=NVAR*NBIT 1 DO L=LC,NVAR*NBIT CHROM(I1,L)=OLD(I2,L)**ENDDO** ENDDO ! MUTATION: ALLOW A SMALL FRACTION OF THE BITS TO MUTATE !

DO I=1,NPOP **!DETERMINE IF A MUTATION OCCURS** CALL RANDOM NUMBER(RAND) IF(RAND.LT.PMUT)THEN!MUTATION OCCURS WHEN TRUE **!SELECT BIT** CALL RANDOM NUMBER(RAND) LBIT=NVAR*NBIT*RAND+0.5 IF(LBIT.LT.1)LBIT=1 IF(LBIT.GT.NVAR*NBIT)LBIT=NVAR*NBIT 1 **! DETERMINE MUTATION** CALL RANDOM NUMBER(RAND) IF(CHROM(I,LBIT))THEN CHROM(I,LBIT)=.FALSE. ELSE CHROM(I,LBIT)=.TRUE. ENDIF ENDIF **ENDDO** ENDDO RETURN END 1 ! DECODE FROM BINARY LOGICAL STRING TO BASE 10 REAL NUMBERS SUBROUTINE DECODE(I) IMPLICIT REAL (A-H, O-Z) **IMPLICIT INTEGER (I-N)** PARAMETER (NPOP=1000,NVAR=5,NBIT=22) LOGICAL CHROM(NPOP,NVAR*NBIT), OLD(NPOP,NVAR*NBIT) COMMON CHROM,OLD,N(NPOP),G(NPOP),F(NPOP),VAR(NVAR) COMMON VOPT(NVAR), FOPT, NGEN, MGEN, PMUT, RAND, IFITTYPE COMMON PABS, T.VO, D.FMDEN, DP, ZMAX, ZMIN, DMFMAX, DMFMIN, DNFMAX, DNFMI N,ANFAMFMAX, ANFAMFMIN,THICKNESSCHK,FMAX,ANFAMFMIN, FMMASSMAX, FMMASSMIN, THICKNESSCHK, DIAMFCHK, DIANFCHK, ARRATIOCHK, MASSMFCHK DO J=1,NVAR VAR(J)=0.0ISTART=(J-1)*NBIT+1 ISTOP=J*NBIT DO L = ISTART, ISTOP IF(CHROM(I,L))THEN VAR(J)=VAR(J)+2.0**(L-(J-1)*NBIT-1)ENDIF ENDDO VAR(J)=VAR(J)/(2.0**NBIT-1.0) **ENDDO** RETURN END ١ ! WRITE RESULTS TO THE SCREEN SO THE USER MAY VIEW THEM

! THIS ROUTINE NEEDS TO BE MODIFIED FOR EACH APPLICATION SUBROUTINE RESULTS IMPLICIT REAL (A-H, O-Z) IMPLICIT INTEGER (I-N) ! PARAMETER (NPOP=1000,NVAR=5,NBIT=22) ! LOGICAL CHROM(NPOP,NVAR*NBIT), OLD(NPOP,NVAR*NBIT) COMMON CHROM,OLD,N(NPOP),G(NPOP),F(NPOP),VAR(NVAR) COMMON VOPT(NVAR),FOPT,NGEN,MGEN,PMUT,RAND,IFITTYPE COMMON VOPT(NVAR),FOPT,NGEN,MGEN,PMUT,RAND,IFITTYPE COMMON PABS,T,VO,D,FMDEN,DP,ZMAX,ZMIN,DMFMAX,DMFMIN,DNFMAX,DNFMI N,ANFAMFMAX, ANFAMFMIN,THICKNESSCHK,FMAX,ANFAMFMIN, FMMASSMAX, FMMASSMIN,THICKNESSCHK,DIAMFCHK, ARRATIOCHK,MASSMFCHK

DIMENSION V(NVAR) !REAL Z,D,PABS,T,VO,FMMASS,FMDEN

REWIND(7)

WRITE(*,*)'MGEN CONVERGENCE FOPT VARIABLES' DO I=1,MGEN READ(7,*,END=10)K,CONV,F1,V WRITE(*,*)K,CONV,F1,V

10 CONTINUE ENDDO

RETURN END

!

FUNCTION FUNC() IMPLICIT REAL (A-H, O-Z) IMPLICIT INTEGER (I-N)

PARAMETER (NPOP=1000,NVAR=5,NBIT=22)

LOGICAL CHROM(NPOP,NVAR*NBIT), OLD(NPOP,NVAR*NBIT) COMMON CHROM,OLD,N(NPOP),G(NPOP),F(NPOP),VAR(NVAR) COMMON VOPT(NVAR),FOPT,NGEN,MGEN,PMUT,RAND,IFITTYPE COMMON PABS,T,VO,D,FMDEN,DP,ZMAX,ZMIN,DMFMAX,DMFMIN,DNFMAX,DNFMI N,ANFAMFMAX, ANFAMFMIN,THICKNESSCHK,FMAX,ANFAMFMIN, FMMASSMAX, FMMASSMIN,THICKNESSCHK,DIAMFCHK,DIANFCHK, ARRATIOCHK,MASSMFCHK

! VARIABLES VAR ARE LIMITED TO A DIMENSIONLESS RANGE OF 0 TO 1
 ! THE ACTUAL VALUES USED IN THE FUNCTION ARE SCALED TO THE SEARCH RANGE

! MEDIA SIZE

IF (THICKNESSCHK.EQ.1) THEN Z=(ZMAX-ZMIN)*VAR(3)+ZMIN

ELSE

Z=ZMIN VAR(3)=0 END IF PI = 3.141592654V = PI*D**2/4*Z

! MEDIUM VOLUME, M3

! MICROFIBERS (MF) IF (DIAMFCHK.EQ.1) THEN

DMF=(DMFMAX-DMFMIN)*VAR(2)+DMFMIN

ELSE

DMF=DMFMIN VAR(2)=0

END IF

DMF = DMF/1000000.0 ! DIAMETER MF, M IF(MASSMFCHK.EQ.1)THEN

FMMASS=(FMMASSMAX-MMASSMIN)*VAR(5)+FMMASSMIN

ELSE

FMMASS=FMMASSMIN VAR(5)=0

END IF

VMF = FMMASS/FMDEN ! VOLUME OF MF, M3 ZMF = VMF*4.0/PI/DMF/DMF! LENGTH OF MF, M AMF = PI*DMF*ZMF ! EXTERNAL AREA OF MF, M2 EMF = VMF/V ! MF VOLUME FRACTION

! NANOFIBERS (NF)

IF (ARRATIOCHK.EQ.1)THEN

ANFAMF=(ANFAMFMAX-ANFAMFMIN)*VAR(4)+ANFAMFMIN ! AREA RATIO OF NF TO MF

ELSE

ANFAMF=ANFAMFMIN VAR(4)=0

END IF

ANF = ANFAMF*AMF ! EXTERNAL AREA NF, M2

IF(DIANFCHK.EQ.1)THEN

DNF=(DNFMAX-DNFMIN)*VAR(1)+DNFMIN

ELSE

DNF=DNFMIN VAR(1)=0 END IF

DNF = DNF/1.0E9 ! DIAMETER OF NF, M ZNF = ANF/PI/DNF ! LENGTH OF NF, M VNF = PI/4.0*DNF**2*ZNF ! VOLUME OF NF, M3 ENF = VNF/V ! NF VOLUME FRACTION **! MEDIA VALUES** ES = ENF + EMF**! FIBER VOLUME FRACTION** E = 1.0 - ES**! FILTER POROSITY** S = 0.1**! LIQUID PHASE VOLUME FRACTION ! OPERATING CONDITIONS (ASSUMES AIR FOR GAS)** VGAS = VO/(1.0-S)/E! PORE AVG GAS VELOCITY, M/S ZLAMBDA=0.231548E-9*T*101.3/PABS ! GAS MEAN FREE PATH, M GMW = 29.0! GAS MOLECULAR WT, KG/KGMOL GR = 0.08205! GAS LAW CONST, ATM*M3/K/KGMOL GDEN = PABS*GMW/101.34/T/GR ! GAS DENSITY, KG/M3 GVIS = 0.019E-3! GAS VISCOSITY, KG/M/S **! PARTICLES** DP = 0.15**! PARTICLE DIAMETER, MICRONS** DP1 = DP/1.0E6**! PARTICLE DIAMETER, M** BOLTK = 1.380660E-23 ! BOLTZMANN CONST, JOULES/K DIFF = BOLTK*T/GVIS/3/PI/DP1 ! PART DIFFUSIV KG/M/S ! BSL2, PG 529, EQ 17.4-3 **! ALPHA CALCULATIONS ! ASSUMES DIFFUSION AND INTERCEPTION DOMINATE** ! REF R.C. BROWN, AIR FILTRATION, PERGAMON, 1993 **! MICROFIBERS** ALPHAMF = 4.0 * EMF/PI/DMF! IDEAL ALPHA MF ZETA = -(0.75+0.5*LOG(EMF))**! HYDRO FACTOR** ! BROWN PG 44 ZKN = 2.0*ZLAMBDA/DMF ! KNUDSEN NO. IF(ZKN.LT.0.01)THEN **! CONTINUUM FLOW** EDRMF = 4.0/ZETA/(DMF**2)*(3.0*DIFF*ZETA*(DMF**2)*PI/8.0/VGAS& +(DP1/2.0)**3)**(2.0/3.0) ! BROWN EQ 4.63 ELSE **! SLIP FLOW** ZPE = VGAS*DMF/DIFF ! PECLET NO. ZETAP = -0.5*LOG(EMF)-0.52+0.64*EMF+1.43*(1.0-EMF)*ZKN ED = 2.7*ZPE**(-2.0/3.0)&*(1.0+0.39*(ZETAP*ZPE)**(-1.0/3.0)*ZKN) R=1+DP1/DMF ER=0.5/ZETAP*(1./R-R+2.*R*LOG(R)+2.86*ZKN*(1.+R)*(R-1)/R) EPRIME=1.24*(R-1.0)**(2./3.)/(ZETAP*ZPE)**0.5 EDRMF = ED + ER + EPRIME ! BROWN EQS 4.64 - 4.68 END IF 1 **! NANOFIBERS** ALPHANF = 4.0 * ENF/PI/DNF! IDEAL ALPHA MF ZETA = -(0.75+0.5*LOG(ENF))**! HYDRO FACTOR** ! BROWN PG 44 ZKN = 2.0*ZLAMBDA/DNF! KNUDSEN NO. IF(ZKN.LT.0.01)THEN **! CONTINUUM FLOW** EDRNF = 4.0/ZETA/DNF**2*(3.0*DIFF*ZETA*DNF**2*PI/8.0/VGAS& +(DP1/2.0)**3)**(2.0/3.0) ! BROWN EQ 4.63 ELSE **! SLIP FLOW**

!

```
ZPE = VGAS*DNF/DIFF
                                         ! PECLET NO.
             ZETAP = -0.5*LOG(ENF)-0.52+0.64*ENF+1.43*(1.0-ENF)*ZKN
             ED = 2.7*ZPE**(-2.0/3.0)\&
             *(1.0+0.39*(ZETAP*ZPE)**(-1.0/3.0)*ZKN)
             R=1+DP1/DNF
             ER=0.5/ZETAP*(1./R-R+2.*R*LOG(R)+2.86*ZKN*(1.+R)*(R-1)/R)
             EPRIME=1.24*(R-1.0)**(2./3.)/(ZETAP*ZPE)**0.5
             EDRNF = ED + ER + EPRIME ! BROWN EQS 4.64 - 4.68
      ENDIF
      ! ALPHA
      ALPHA = EDRNF*ALPHANF + EDRMF*ALPHAMF
! FI CALCULATIONS (CHASE NOTES PP 79-81)
      1
      ! MICROFIBERS
      ZKN = 2.0*ZLAMBDA/DMF
      IF(ZKN.LT.0.01)THEN
                                  ! CONTINUUM
             FIMF=4.0*GVIS*PI*VGAS/(-0.5*LOG(EMF)-0.738+EMF)
                    1
      ELSE IF(ZKN.LT.0.25)THEN
                                  ! SLIP
             FIMF=4.0*GVIS*PI*VGAS*(1.0+1.996*ZKN)&
             /(-0.5*LOG(EMF)-0.75+EMF-0.25*EMF**2+1.996*ZKN&
             *(-0.5*LOG(EMF)-0.25*(1.0-EMF**2)))
             1
      ELSE IF(ZKN.GT.10) THEN
                                  ! MOLECULAR
             FIMF=7.194*GVIS*VGAS/ZKN
      1
      ELSE
                                  ! INTERMEDIATE
             FI25=4.0*GVIS*PI*VGAS*(1.0+1.996*0.25)&
             /(-0.5*LOG(EMF)-0.75+EMF-0.25*EMF**2+1.996*0.25&
             *(-0.5*LOG(EMF)-0.25*(1.0-EMF**2)))
             FI10=7.194*GVIS*VGAS/10
             FIMF=(FI10-FI25)/(10.-0.25)*(ZKN-0.25)+FI25
             END IF
             1
      ! NANOFIBERS
      ZKN = 2.0*ZLAMBDA/DNF
      IF(ZKN.LT.0.01)THEN
                                  ! CONTINUUM
             FINF=4.0*GVIS*PI*VGAS/(-0.5*LOG(ENF)-0.738+ENF)
             ELSE IF(ZKN.LT.0.25)THEN
                                ! SLIP
             FINF=4.0*GVIS*PI*VGAS*(1.0+1.996*ZKN)&
             /(-0.5*LOG(ENF)-0.75+ENF-0.25*ENF**2+1.996*ZKN&
             *(-0.5*LOG(ENF)-0.25*(1.0-ENF**2)))
      ELSE IF(ZKN.GT.10) THEN
                                  ! MOLECULAR
             FINF=7.194*GVIS*VGAS/ZKN
      ELSE
                                  ! INTERMEDIATE
             FI25=4.0*GVIS*PI*VGAS*(1.0+1.996*0.25)&
             /(-0.5*LOG(ENF)-0.75+ENF-0.25*ENF**2+1.996*0.25&
             *(-0.5*LOG(ENF)-0.25*(1.0-ENF**2)))
             FI10=7.194*GVIS*VGAS/10
             FINF= (FI10-FI25)/(10.-0.25)*(ZKN-0.25)+FI25
```

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END IF PGRAD=4.0/PI*(EMF*FIMF/DMF**2+ENF*FINF/DNF**2) PGRAD=4.0/PI*(EMF*FIMF/DMF*FIMF/DMF*FIMF/DMF**2+ENF*FIMF/DMF*FIMF/DMF**2+ENF*FIMF/DMF*FIMF/DMF**2+ENF*FIMF/DMF**2+ENF*FIMF/DMF*FIMF/DMF**2+ENF*FIMF/DMF*FIMF/DMF*FIMF/DMF*FIMF/DMF*FIMF/DMF*FIMF/DMF*FIMF/DMF*FIMF/DMF*FIMF/DMF*FIMF/DMF*FIMF/DMF*FIMF/DMF*FIMF/DMF*FIMF/DMF*FIMF/DMF*FIMF*FIMF/DMF*FI

APPENDIX B

VISUAL BASIC PROGRAM

The user interface is written in visual basic program. The input from the user is sent to fortran program and the calculation is done in the fortran executable file and the results is returned back in visual basic interface.

PRIVATE SUB START_CLICK() 'THESE ARE THE OPTIMUM PARAMETERS 'GETTING THE VALUE FROM TEXT

THICKNESS1 = THICKNESS.TEXT

'RETURNS AN INTEGER SPECIFYING THE STARTING POSITION OF OCCURENCE OF STRING '-' WITHIN ANOTHER SPACEPOSZ = INSTR(THICKNESS1, "-")

'MID FUNCTION WILL EXTRACT THE SUBSTRING THE STRING FROM POSITION 1 TO THE STRING POSITION WITHSPACEPOZ-1 ZMIN1 = MID(THICKNESS1, 1, SPACEPOSZ - 1)

'THIS WILL EXTRACT THE STRING FROM SPACEPOSZ+1 TO END OF THE STRING AND STORE IT IN VARIABLE

```
ZMAX1 = MID(THICKNESS1, SPACEPOSZ + 1)
DIAMF1 = DIAMF.TEXT
SPACEPOSMF = INSTR(DIAMF1, "-")
DMFMIN1 = MID(DIAMF1, 1, SPACEPOSMF - 1)
DMFMAX1 = MID(DIAMF1, SPACEPOSMF + 1)
DIANF1 = DIANF.TEXT
SPACEPOSNF = INSTR(DIANF1, "-")
DNFMIN1 = MID(DIANF1, 1, SPACEPOSNF - 1)
DNFMAX1 = MID(DIANF1, SPACEPOSNF + 1)
AREARATIO1 = AREARATIO.TEXT
SPACEPOSAR = INSTR(AREARATIO1, "-")
ARMIN1 = MID(AREARATIO1, 1, SPACEPOSAR - 1)
ARMAX1 = MID(AREARATIO1, SPACEPOSAR + 1)
MASSMF1 = MASSMF.TEXT
SPACEPOSMMF = INSTR(MASSMF1, "-")
MMFMIN1 = MID(MASSMF1, 1, SPACEPOSMMF - 1)
MMFMAX1 = MID(MASSMF1, SPACEPOSMMF + 1)
```

TEXT2.TEXT = ""

```
TEXT7.TEXT = " "
MSCHART1.VISIBLE = FALSE
VIEWRESULTS.ENABLED = FALSE
SAVERESULTS.ENABLED = FALSE
VIEWPLOTS.ENABLED = FALSE
'UNIT CONVERSION
IF COMBO1(0).TEXT = "PSI" THEN
 PRESSURE1 = VAL(PRESSURE(0).TEXT) / 0.145
ELSE
 PRESSURE1 = VAL(PRESSURE(0).TEXT)
END IF
IF COMBO2(0).TEXT = "C" THEN
  TEMPERATURE1 = VAL(TEMPERATURE(0).TEXT) + 273.15
ELSE
 TEMPERATURE1 = VAL(TEMPERATURE(0).TEXT)
END IF
IF COMBO3(0).TEXT = "CM/SEC" THEN
 FACEVELOCITY1 = VAL(FACEVELOCITY(0).TEXT) / 100
ELSE
 FACEVELOCITY1 = VAL(FACEVELOCITY(0).TEXT)
END IF
IF COMBO4(0).TEXT = "CM" THEN
 DIAFILTER1 = VAL(DIAFILTER(0).TEXT) / 100
ELSE
 DIAFILTER1 = VAL(DIAFILTER(0).TEXT)
END IF
IF COMBO5(0).TEXT = "G/CM3" THEN
 DENSITY1 = VAL(DENSITY(0).TEXT) * 1000
ELSE
 DENSITY1 = VAL(DENSITY(0).TEXT)
END IF
IF COMBO9.TEXT = "M" THEN
 DIAP1 = VAL(DIAP(1).TEXT) / 0.00001
ELSE
 DIAP1 = VAL(DIAP(1).TEXT)
END IF
 THICKNESSCHK1 = THICKNESSCHK.VALUE
 ARRATIOCHK1 = ARRATIOCHK.VALUE
 DIANFCHK1 = DIANFCHK.VALUE
 DIAMFCHK1 = DIAMFCHK.VALUE
 MASSMFCHK1 = MASSMFCHK, VALUE
 IF THICKNESSCHK.VALUE = 0 THEN
   TEXT1.VISIBLE = TRUE
   THICKNESS.VISIBLE = FALSE
 IF COMBO6.TEXT = "CM" THEN
   ZMIN1 = VAL(TEXT1.TEXT) / 100
 ELSE
   ZMIN1 = VAL(TEXT1.TEXT)
```

```
END IF
    ZMAX1 = 0
 ELSE
   THICKNESS.VISIBLE = TRUE
   TEXT1.VISIBLE = FALSE
  END IF
IF ARRATIOCHK.VALUE = 0 THEN
   TEXT4.VISIBLE = TRUE
   AREARATIO.VISIBLE = FALSE
   ARMIN1 = TEXT4.TEXT
   ARMAX1 = 0
 ELSE
   AREARATIO.VISIBLE = TRUE
   TEXT4.VISIBLE = FALSE
 END IF
 IF DIAMFCHK.VALUE = 0 THEN
   TEXT6.VISIBLE = TRUE
   DIAMF.VISIBLE = FALSE
 IF COMBO7.TEXT = "M" THEN
    DMFMIN1 = VAL(TEXT6.TEXT) / 0.00001
 ELSE
   DMFMIN1 = VAL(TEXT6.TEXT)
 END IF
   DMFMAX1 = 0
 ELSE
   DIAMF.VISIBLE = TRUE
   TEXT6.VISIBLE = FALSE
 END IF
 IF DIANFCHK.VALUE = 0 THEN
   TEXT3.VISIBLE = TRUE
   DIANF.VISIBLE = FALSE
  IF COMBO8.TEXT = "M" THEN
   DNFMIN1 = VAL(TEXT3.TEXT) / 0.00000001
 ELSE
    DNFMIN1 = VAL(TEXT3.TEXT)
 END IF
    DNFMAX1 = 0
 ELSE
   DIANF.VISIBLE = TRUE
   TEXT3.VISIBLE = FALSE
 END IF
 IF MASSMFCHK.VALUE = 0 THEN
    TEXT5.VISIBLE = TRUE
    MASSMF.VISIBLE = FALSE
  IF COMBO10.TEXT = "G" THEN
     MMFMIN1 = TEXT5.TEXT / 1000
 ELSE
     MMFMIN1 = TEXT5.TEXT
 END IF
    MMFMAX1 = 0
 ELSE
   MASSMF.VISIBLE = TRUE
```

TEXT5.VISIBLE = FALSE END IF

'GENETIC ALGORITHM PARAMETERS

```
POPULATION1 = POPULATION.TEXT
GENERATION1 = GENERATION.TEXT
MUTATION1 = MUTATION.TEXT
CONVERGENCE1 = CONVERGENCE.TEXT
```

```
IF THICKNESSCHK1 = 0 THEN
  Z = ZMIN1
ELSE
  Z = ZMIN1
  Z = ZMAX1
END IF
IF DIAMFCHK1 = 0 THEN
 DMF = DMFMIN1
ELSE
 DMF = DMFMIN1
 DMF = DMFMAX1
END IF
IF MASSMFCHK1 = 0 THEN
  FMMASS = MMFMIN1
ELSE
 FMMASS = MMFMIN1
 FMMASS = MMFMAX1
END IF
IF ARRATIOCHK1 = 0 THEN
  ANFAMF = ARMIN1
ELSE
  ANFAMF = ARMIN1
  ANFAMF = ARMAX1
END IF
IF DIANFCHK1 = 0 THEN
  DNF = DNFMIN1
ELSE
 DNF = DNFMIN1
 DNF = DNFMAX1
END IF
 DP = DIAP1
 D = DIAFILTER1
 FMDEN = DENSITY1
 PI = 3.141592654
  VO = FACEVELOCITY1
  V = PI * D ^ 2 / 4 * Z ' MEDIUM VOLUME M3
 'MICROFIBERS (MF)
 DMF = DMF / 1000000 ' DIAMETER MF, M
```

VMF = FMMASS / FMDEN ' VOLUME OF MF, M3 ZMF = VMF * 4 / PI / DMF / DMF ' LENGTH OF MF, M AMF = PI * DMF * ZMF ' EXTERNAL AREA OF MF, M2 EMF = VMF / V 'MF VOLUME FRACTION ANF = ANFAMF * AMF ' EXTERNAL AREA NF, M2 DNF = DNF / 1000000000 ' DIAMETER OF NF, M ZNF = ANF / PI / DNF ' LENGTH OF NF, M VNF = PI / 4 * DNF ^ 2 * ZNF ' VOLUME OF NF, M3 ENF = VNF / V 'NF VOLUME FRACTION ' 'MEDIA VALUES ES = ENF + EMF ' FIBER VOLUME FRACTION E = 1 - ES ' FILTER POROSITY

IF E < 0 THEN

MSGBOX " CHECK THE PARAMETERS : POROSITY " & FORMAT(E, "#.00E-00") PRESSURE(0).SETFOCUS

'OPENING A TEXT FILE TO STORE THE INPUT DATA

ELSE

OPEN "C:\INPUTVAR.TXT" FOR OUTPUT AS #2

PRINT #2, PRESSURE1, TEMPERATURE1, FACEVELOCITY1, DIAFILTER1, DENSITY1, DIAP1, THICKNESSCHK1, ZMIN1, ZMAX1, DIAMFCHK1, DMFMIN1, DMFMAX1, DIANFCHK1, DNFMIN1, DNFMAX1, ARRATIOCHK1, ARMIN1, ARMAX1, MASSMFCHK1, MMFMIN1, MMFMAX1, GENERATION1, MUTATION1, CONVERGENCE1 CLOSE #2

'FORTRAN EXECUTABLE FILE

W\$ = "C:\GAVBCONV.EXE" 'USED SHELL FUNCTION TO RUN THE FORTRAN EXECUTABLE FILE

VIEWRESULTS.ENABLED = FALSE LABEL11.CAPTION = "PROGRAM IS RUNNING" CALL SHELLANDWAIT(W\$, 8000) LABEL11.CAPTION = "PROGRAM IS STOPPED" VIEWRESULTS.ENABLED = TRUE

END IF END SUB

OPTION EXPLICIT

PRIVATE DECLARE FUNCTION OPENPROCESS LIB "KERNEL32" _ (BYVAL DWDESIREDACCESS AS LONG, BYVAL BINHERITHANDLE AS LONG, _ BYVAL DWPROCESSID AS LONG) AS LONG

PRIVATE DECLARE FUNCTION GETEXITCODEPROCESS LIB "KERNEL32" _ (BYVAL HPROCESS AS LONG, LPEXITCODE AS LONG) AS LONG

PRIVATE CONST STATUS_PENDING = &H103& PRIVATE CONST PROCESS_QUERY_INFORMATION = &H400 'DIM VALUE1 AS STRING

PUBLIC FUNCTION SHELLANDWAIT(EXEFULLPATH AS STRING, _ OPTIONAL TIMEOUTVALUE AS LONG = 0) AS BOOLEAN

DIM LINST AS LONG DIM LSTART AS LONG DIM LTIMETOQUIT AS LONG DIM SEXENAME AS STRING DIM LPROCESSID AS LONG DIM LEXITCODE AS LONG DIM BPASTMIDNIGHT AS BOOLEAN

DIM I AS INTEGER ON ERROR GOTO ERRORHANDLER

LSTART = CLNG(TIMER) SEXENAME = EXEFULLPATH

'DEAL WITH TIMEOUT BEING RESET AT MIDNIGHT IF TIMEOUTVALUE > 0 THEN IF LSTART + TIMEOUTVALUE < 86400 THEN LTIMETOQUIT = LSTART + TIMEOUTVALUE

ELSE LTIMETOQUIT = (LSTART - 86400) + TIMEOUTVALUE BPASTMIDNIGHT = TRUE 'MSGBOX "PROGRAM IS RUNNING" END IF END IF

LINST = SHELL(SEXENAME, VBMINIMIZEDNOFOCUS)

'LINST = SHELL(SEXENAME, VBMAXIMIZEDFOCUS) LPROCESSID = OPENPROCESS(PROCESS_QUERY_INFORMATION, FALSE, LINST)

DO

```
CALL GETEXITCODEPROCESS(LPROCESSID, LEXITCODE)
DOEVENTS
IF TIMEOUTVALUE AND TIMER > LTIMETOQUIT THEN
IF BPASTMIDNIGHT THEN
IF TIMER < LSTART THEN EXIT DO
ELSE
EXIT DO
END IF
```

END IF

LOOP WHILE LEXITCODE = STATUS_PENDING

MSGBOX "COMPLETED EXECUTING THE MODEL"

SHELLANDWAIT = TRUE

ERRORHANDLER: SHELLANDWAIT = FALSE EXIT FUNCTION END FUNCTION

PRIVATE SUB VIEWPLOTS_CLICK() DIM SFILE AS STRING, SMSG AS STRING DIM VAL1() AS SINGLE, VAL2() AS VARIANT, VAL3() AS SINGLE, VAL4() AS SINGLE DIM VAL5() AS SINGLE, VAL6() AS VARIANT, VAL7() AS SINGLE, VAL8() AS SINGLE DIM FIRST AS SINGLE DIM IIDX AS LONG DIM CONV AS SINGLE DIM K AS INTEGER 'DIM DATATHK(0 TO 10) AS STRING

DIM ARRDATA(100, 1 TO 2) DIM I AS INTEGER, COUNT AS INTEGER DIM MAXN1, MIN1 DIM MAXN2, MIN2 COMB014.CLEAR COMB015.CLEAR MSCHART1.VISIBLE = TRUE

'OPENING AN EXTERNAL FILE WHERE THE OUTPUT IS STORED. 'THE CALCULATION IS DONE IN FORTRAN FILE AND THE OUTPUT IS STORED IN GA.DAT FILE.

SFILE = "C: GA.TXT"

'READ ALL THE VARIABLES UNTIL END OF FILE IS REACHED

IIDX = 0 OPEN SFILE FOR INPUT AS #1 DO WHILE NOT EOF(1) REDIM PRESERVE VAL1(IIDX) REDIM PRESERVE VAL2(IIDX) REDIM PRESERVE VAL3(IIDX) REDIM PRESERVE VAL4(IIDX) REDIM PRESERVE VAL5(IIDX) REDIM PRESERVE VAL6(IIDX) REDIM PRESERVE VAL8(IIDX)

INPUT #1, VAL1(IIDX), VAL2(IIDX), VAL3(IIDX), VAL4(IIDX), VAL5(IIDX), VAL6(IIDX), VAL7(IIDX), VAL8(IIDX)

IIDX = IIDX + 1

LOOP

CLOSE FOR IIDX = LBOUND(VAL1) TO UBOUND(VAL1) CONV = VAL2(IIDX)

```
VAL6(IIDX) = (ZMAX1 - ZMIN1) * VAL6(IIDX) + ZMIN1
VAL5(IIDX) = (DMFMAX1 - DMFMIN1) * VAL5(IIDX) + DMFMIN1
VAL4(IIDX) = (DNFMAX1 - DNFMIN1) * VAL4(IIDX) + DNFMIN1
VAL7(IIDX) = (ARMAX1 - ARMIN1) * VAL7(IIDX) + ARMIN1
VAL8(IIDX) = (MMFMAX1 - MMFMIN1) * VAL8(IIDX) + MMFMIN1
```

```
SMSG = SMSG & _VAL1(IIDX) & " * VAL2(IIDX) & " * & VAL3(IIDX) & " * & VAL4(IIDX) & " * & VAL4(IIDX) & " * & VAL5(IIDX) & " * & VAL6(IIDX) & " * & VAL7(IIDX) & " * & VAL7(IIDX) & " * & VAL8(IIDX) & * * & VAL8(IIDX) & * * & VAL1(IIDX)) COMB014.ADDITEM (VAL1(IIDX))
COMB015.ADDITEM (VAL2(IIDX))
NEXT IIDX
COUNT = COMB014.LISTCOUNT
MSCHART1.REFRESH
FOR I = 2 TO COUNT
```

ARRDATA(I, 1) = COMBO14.LIST(I - 1)ARRDATA(I, 2) = COMBO15.LIST(I - 1)

NEXT I

```
MAXN1 = COMBO15.LIST(1)
MAXN2 = COMBO14.LIST(1)
FOR I = 2 TO COUNT
IF MAXN1 < VAL(COMBO15.LIST(I)) THEN
MAXN1 = COMBO15.LIST(I)
END IF
```

IF MAXN2 < VAL(COMBO14.LIST(I)) THEN MAXN2 = COMBO14.LIST(I) END IF NEXT I

MSCHART1.VISIBLE = TRUE

```
MSCHART1.PLOT.AXIS(VTCHAXISIDX).AXISTITLE = "GENERATION"
MSCHART1.PLOT.AXIS(VTCHAXISIDY).AXISTITLE = "CONVERGENCE"
WITH MSCHART1.PLOT.AXIS(VTCHAXISIDY).VALUESCALE
.AUTO = FALSE
.MINIMUM = 0.000000001
.MAXIMUM = MAXN1
```

```
MSCHART1.PLOT.AXIS(VTCHAXISIDY).VALUESCALE.MAJORDIVISION = 0.001
MSCHART1.PLOT.AXIS(VTCHAXISIDY).VALUESCALE.MINORDIVISION = 0.0002
MSCHART1.PLOT.AXIS(VTCHAXISIDY).AXISSCALE.HIDE = FALSE
```

```
END WITH
WITH MSCHART1.PLOT.AXIS(VTCHAXISIDX).VALUESCALE
.AUTO = FALSE
.MINIMUM = 1
.MAXIMUM = MAXN2
MSCHART1.PLOT.AXIS(VTCHAXISIDX).VALUESCALE.MAJORDIVISION = 2
MSCHART1.PLOT.AXIS(VTCHAXISIDX).VALUESCALE.MINORDIVISION = 0.4
```

MSCHART1.PLOT.AXIS(VTCHAXISIDX).AXISSCALE.HIDE = FALSE END WITH MSCHART1.CHARTDATA = ARRDATA MSCHART1.PLOT.UNIFORMAXIS = FALSE IF (THICKNESSCHK.VALUE = 0) THEN MSGBOX "THICKNESS ENABLED" COMBO13.REMOVEITEM (1) END IF END SUB